

Molecular sets and representations of chemical reactions

A uni-molecular chemical reaction is represented by the [natural](#)

[transformations](#) $\eta : h^A \longrightarrow h^B$, through the following [commutative diagram](#):

$$\begin{array}{ccc} h^A(A) = Hom(A, A) & \xrightarrow{\eta_A} & h^B(A) = Hom(B, A) \\ \downarrow h^A(t) & & \downarrow h^B(t) \\ h^A(B) = Hom(A, B) & \xrightarrow{\eta_B} & h^B(B) = Hom(B, B) \end{array} \quad (0.1)$$

with the states of molecular sets $A_u = a_1, \dots, a_n$ and $B_u = b_1, \dots, b_n$ being represented by certain endomorphisms in $Hom(A, A)$ and $Hom(B, B)$, respectively. In

general, molecular sets M_S are defined as finite sets whose elements are molecules defined in terms of their molecular [observables](#) that are specified next. One need to define first the [concept](#) of a molecular class variable. A molecular class variable, or *m.c.v* is defined as a

family of molecular sets $[M_S]_{i \in I}$, with I being an indexing set, or class, defining the molecular range of variation of the *m.c.v*. Most applications in Physics, Chemistry or Biochemistry require that I is a finite set, (that is, without any sub-classes). A homomorphism of molecular sets $M_t : M_S \rightarrow M_S$, $t \in T$, with t being real time values, is defined as a time-dependent mapping or [function](#) $M_S(t)$ also called a M_t molecular transformation.

An *m.c.v*. observable of B , characterizing the products of chemical [type](#) “B” of a chemical

reaction is defined as a [morphism](#):

$$\gamma : Hom(B, B) \longrightarrow \mathfrak{R},$$

where $\mathfrak{R}$ is the set or [field](#) of real numbers. This mcv-observable is subject to the following [commutativity](#) conditions:

$$\begin{array}{ccc} Hom(A, A) & \xrightarrow{f} & Hom(B, B) \\ \downarrow \epsilon & & \downarrow \gamma \\ Hom(A, A) & \xrightarrow{\delta} & R, \end{array} \quad (0.2)$$

with $c : A_u^* \longrightarrow B_u^*$, and A_u^*, B_u^* being, respectively, specially prepared fields of states of the molecular sets A_u and B_u within a measurement uncertainty range, Δ , which is determined by Heisenberg's uncertainty [relation](#), or the [commutator](#) of the observable [operators](#) involved, such as $[A^*, B^*]$, associated with the observable A of molecular set A_u , and respectively, with the observable B of molecular set B_u , in the case of a molecular set A_u interacting with molecular set B_u .

With these concepts and preliminary data one can now define the [category of molecular sets](#) and their transformations as follows.

Category of molecular sets and their transformations

Definition 0.1 The category of molecular sets is defined as the [category](#) C_M whose [objects](#) are molecular sets M_S and whose morphisms are molecular transformations M_t .

Remark 0.1 This is a mathematical [representation](#) of chemical reaction [systems](#) in terms of molecular sets that vary with time (or *msv*'s), and their transformations as a result of

diffusion, [collisions](#), and chemical reactions.

Bibliography

- 1 Bartholomay, A. F.: 1960. Molecular Set Theory. A mathematical representation for chemical reaction mechanisms. Bull. Math. Biophys., 22: 285-307.
- 2 Bartholomay, A. F.: 1965. Molecular Set Theory: II. An aspect of biomathematical theory of sets., Bull. Math. Biophys. 27: 235-251.
- 3 Bartholomay, A.: 1971. Molecular Set Theory: III. The Wide-Sense Kinetics of Molecular Sets ., Bulletin of Mathematical Biophysics, 33: 355-372.
- 4 Baianu, I. C.: 1983, Natural Transformation Models in Molecular Biology., in Proceedings of the SIAM Natl. Meet., Denver, CO.; Eprint at cogprints.org with No. 3675.
- 4 Baianu, I.C.: 1984, A Molecular-Set-Variable Model of Structural and Regulatory Activities in Metabolic and Genetic Networks FASEB Proceedings 43, 917.

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